

Effect of weak impurities on electronic properties of graphene: Functional renormalization-group analysis

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We consider an effect of weak impurities on the electronic properties of graphene within the functional renormalization-group approach. The energy dependences of the electronic self-energy and density of states near the neutrality point are discussed. Depending on the symmetry of the impurities, the electronic damping Γ and density of states ρ can deviate substantially from those given by the self-consistent Born approximation. We investigate the crossover from the results of the self-consistent Born approximation, which are valid far from the neutrality point to the strong-coupling (diffusive) regime near the neutrality point. For impurities, which are diagonal in both valley and sublattice indices, we obtain a finite density of states at the Fermi level with values which are much bigger than the result of the self-consistent Born approximation.

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Graphene is a two-dimensional system with Dirac electronic dispersion that possesses unique properties. In particular, the electronic properties of graphene near the neutrality point remain a challenging problem in condensed-matter physics. Unlike many two-dimensional systems, the conductivity remains finite at the neutrality point.¹ Although the density of states (DOS) for systems with Dirac dispersion is expected to vanish at the neutrality point, a finite DOS at the corresponding position of the Fermi level was observed experimentally in graphene.²

The electronic properties of graphene are expected to be strongly influenced by impurities. Although the chiral disorder does not lead to localization,^{3,4} this particular type of disorder is realized only for infinitely strong impurities (e.g., vacancies). The effect of strong impurities was intensively investigated within both analytical⁵ and numerically exact approaches.^{6,7}

At the same time, even weak impurities may have a nontrivial effect on the electronic properties of graphene. In particular, the chiral disorder of the CI symmetry class was argued to yield an energy dependence $\varepsilon^{1/7}$ of the density of states near the neutrality point.⁸ This result is distinctly different from that of the self-consistent Born approximation (SCBA),⁹ considering only multiple scattering of electrons on the same impurity, which enlightens the importance of interimpurity scattering processes. It was also shown in Ref. 4 that for long-range disorder, which is diagonal in both valley and sublattice spaces, SCBA predicts a much smaller damping of electrons close to the neutrality point than that expected from other approaches.

The standard renormalization-group (RG) approach of Ref. 4 allows one to describe interimpurity scattering, but it only treats the ballistic regime of the flow. In particular, this approach yields a divergence of the vertices at some critical length scale, which does not allow one to describe the crossover to the strong-coupling (diffusive) regime. Investigation of the diffusive regime represents, however, an important problem, since it allows one to describe the physical properties in the range of fillings close to the neutrality point. Although some results for the density of states and conductivity were obtained within the nonlinear-sigma model approach (see, e.g., Refs. 4, 8, and 10 and references therein), it is interesting to perform the

analysis starting from the weak-coupling point of view, which may allow one to treat both the strong-coupling (diffusive) regime of the flow and the crossover from the ballistic to diffusive regime.

In this Rapid Communication we investigate the effect of long-range and chiral potential impurities on the electronic properties of graphene within the recently proposed Wick-ordered functional renormalization-group (fRG) scheme,^{11–13} allowing the treatment of self-energy effects beyond the leading order of perturbation theory.

We consider a quartic interaction between Dirac fermions due to averaged potential impurity scattering. Assuming only second-order cumulants are important (i.e., the impurity potentials are substantially weak) the corresponding action reads^{4,14}

$$S = \int d^2x \left[\int d\tau \bar{\psi} (\gamma_\mu \partial_\mu) \psi - \frac{1}{2} n_{\text{imp}} \sum_l T_l^2 \int d\tau \int d\tau' (\bar{\psi}_\tau M_l \psi_\tau) (\bar{\psi}_{\tau'} M_l \psi_{\tau'}) \right], \quad (1)$$

where $\mu = 0, 1, 2$, $\partial = (\partial_\tau, v_F \partial_x, v_F \partial_y)$, $\bar{\psi} = \psi^\dagger \gamma_0$, and γ_μ are the Dirac matrices, e.g.,

$$\gamma_0 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}, \quad \gamma_a = \begin{pmatrix} \sigma_a & 0 \\ 0 & -\sigma_a \end{pmatrix}, \quad (2)$$

where $a = 1, 2$, and σ_i are the Pauli matrices. The quadratic part of the action (1) represents the continuum limit of the microscopic tight-binding model (see, e.g., Refs. 4 and 14) and corresponds to the representation $\psi = \{\psi_A^1, \psi_B^1, \psi_B^2, -\psi_A^2\}$ (ψ_s^m is an annihilation operator for the electron in valley m and sublattice s). The quantities T_l represent scattering amplitudes (impurity potentials) in different channels; the latter are described by 4×4 matrices M_l , belonging to a linearly independent set of complex matrices with $(\gamma_0 M_l)^2 = I$ (I is the identity matrix). The interaction in Eq. (1) is obtained after averaging over impurity positions with $\langle U_l(\mathbf{x}) U_l(\mathbf{x}') \rangle = n_{\text{imp}} T_l^2 \delta^{(2)}(\mathbf{x} - \mathbf{x}')$, and n_{imp} is the impurity concentration. Equation (1) neglects higher than second-order scattering processes on the same impurity,

which implies that this equation is applicable in the limit of weak impurities, $2\pi n_{\text{imp}}[T_l/(2\pi v_F)]^n \ll 1$ for $n \geq 1$.

The mean-field (self-consistent Born) approximation for the model (1) yields for the fermionic self-energy $\hat{\Sigma}^\varepsilon$ (see, e.g., Ref. 4 and references therein),

$$\hat{\Sigma}^\varepsilon = -n_{\text{imp}} \sum_{\mathbf{k}, l} T_l^2 M_l \frac{1}{\gamma_0 \varepsilon - \hat{\Sigma}^\varepsilon + i v_F \gamma_a k_a} M_l. \quad (3)$$

Taking into account that $(M_l \gamma_0)^2 = I$, the solution to this equation has the form $\hat{\Sigma}^\varepsilon = \gamma_0 \Sigma(\varepsilon)$ with

$$\Sigma(\varepsilon) = \frac{U^2 n_{\text{imp}}}{4\pi v_F^2} [\varepsilon - \Sigma(\varepsilon)] \ln \frac{-(v_F \Lambda_{\text{uv}})^2}{[\varepsilon - \Sigma(\varepsilon)]^2}, \quad (4)$$

where $U^2 = \sum_l T_l^2$, and Λ_{uv} is an ultraviolet momentum cutoff. At $\varepsilon \rightarrow 0$ Eq. (4) yields⁴

$$\Sigma(0) = -i\Gamma, \quad \Gamma \simeq \Lambda_{\text{uv}} v_F e^{-2\pi v_F^2/(n_{\text{imp}} U^2)}. \quad (5)$$

Note that the exponential smallness of Γ in graphene in the limit of weak impurities is due to vanishing of the density of states of the pure system at the Fermi level. The density of states of the impure system at the Fermi level in SCBA reads⁴

$$\rho(0) = \frac{4\Gamma}{\pi n_{\text{imp}} U^2}. \quad (6)$$

The renormalization group. To treat the effect of weak impurities beyond SCBA, we apply the recently proposed Wick-ordered functional renormalization-group scheme^{11–13} by considering the sharp momentum cutoff of the electronic propagator in the form

$$C_\Lambda = (\gamma_0 \varepsilon - \hat{\Sigma}_\Lambda^\varepsilon + i v_F \gamma_a k_a)^{-1} \theta(|\mathbf{k}| - \Lambda), \quad (7)$$

where Λ is the cutoff parameter. The corresponding single-scale propagator reads

$$\begin{aligned} S_\Lambda &= -\dot{C}_\Lambda + C_\Lambda \hat{\Sigma}_\Lambda^\varepsilon C_\Lambda \\ &= (\gamma_0 \varepsilon - \hat{\Sigma}_\Lambda^\varepsilon + i v_F \gamma_a k_a)^{-1} \delta(|\mathbf{k}| - \Lambda), \end{aligned} \quad (8)$$

where the dot stands for the derivative over Λ . Following Refs. 12 and 13, we choose the Wick-ordering propagator in the form, which is complementary to C_Λ ,

$$D_\Lambda = (\gamma_0 \varepsilon - \hat{\Sigma}_\Lambda^\varepsilon + i v_F \gamma_a k_a)^{-1} \theta(\Lambda - |\mathbf{k}|). \quad (9)$$

In the renormalization-group approach we have the contribution of three different channels to the vertex renormalization. The replica trick requires that the diagrams with closed loops (i.e., those containing summations over a number of fermion species) should be excluded from the diagram technique. The corresponding fRG equations for the vertex $V_{i_1 \dots i_4}^{\varepsilon \varepsilon'}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ and the self-energy $\hat{\Sigma}_{i_1 i_3 \Lambda}^\varepsilon$ ($i_{1,2}, \mathbf{k}_{1,2}$ and $i_{3,4}, \mathbf{k}_{3,4}$ correspond to valley-sublattice indices and momenta of the incoming and outgoing particles, and ε and ε' are the energies of the interacting particles) are presented in the Supplemental Material¹⁵ and are shown diagrammatically in Fig. 1.

To solve the fRG equations numerically we decompose the vertex into the contributions of particle-hole direct and crossed (ph and ph1), and particle-particle (pp) channels, similarly to Ref. 16,

$$\begin{aligned} V_{i_1 \dots i_4}^{\varepsilon \varepsilon'}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &= V_{i_1 \dots i_4}^{\varepsilon \varepsilon', \text{ph}}(\mathbf{k}_3 - \mathbf{k}_2) + V_{i_1 \dots i_4}^{\varepsilon \varepsilon', \text{ph1}}(\mathbf{k}_1 - \mathbf{k}_3) \\ &\quad + V_{i_1 \dots i_4}^{\varepsilon \varepsilon', \text{pp}}(\mathbf{k}_1 + \mathbf{k}_2). \end{aligned} \quad (10)$$

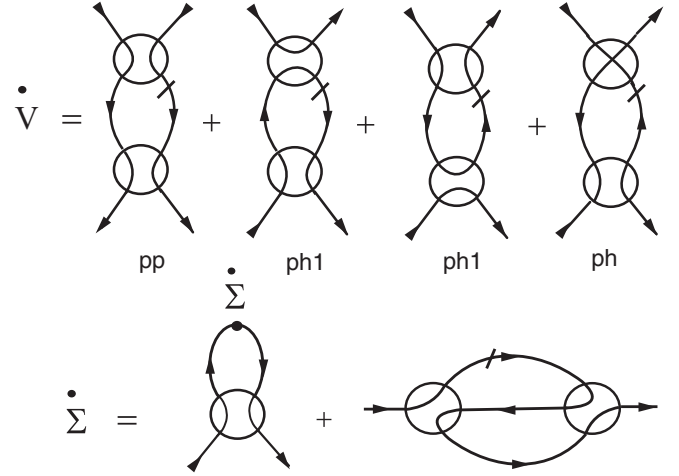


FIG. 1. The diagrammatic form of the fRG equations for the interaction vertices and self-energy. Solid lines with dashes correspond to the single-scale propagator, Eq. (8), and the other solid lines connecting vertices correspond to the Wick propagator (9). The lines inside the vertices connect the legs with the same replica index.

Assuming that the disorder is time-reversal invariant, we also use symmetries of the interaction $V_{i_1 \dots i_4}^{\varepsilon \varepsilon', \text{ph}}(\mathbf{q}) = T_{i_2 i_2'} V_{i_1 i_1' i_3 i_3'}^{\varepsilon \varepsilon', \text{pp}}(\mathbf{q}) T_{i_4 i_4'}$, $V_{i_1 \dots i_4}^{\varepsilon \varepsilon', \text{ph1}}(\mathbf{q}) = T_{i_2 i_2'} V_{i_1 i_1' i_3 i_3'}^{\varepsilon \varepsilon', \text{ph1}}(\mathbf{q}) T_{i_4 i_4'}$, where $T = i\gamma_1 \gamma_3$ is the time-inversion matrix, $\gamma_3 = \begin{pmatrix} 0 & iI \\ -iI & 0 \end{pmatrix}$, and put $\varepsilon' = \varepsilon$, since we consider only the retarded channel of electronic scattering. The initial conditions for the fRG equations read $V_{i_1 \dots i_4}^{\varepsilon \varepsilon} |_{\Lambda = \Lambda_{\text{uv}}} = n_{\text{imp}} \sum_l T_l^2 M_l^{i_1 i_3} M_l^{i_2 i_4}$, $\hat{\Sigma}_{\Lambda = \Lambda_{\text{uv}}}^\varepsilon$ is determined by the Eq. (4).

Results. Below we consider the long-range disorder, diagonal in both sublattice and valley subspaces ($2 \times \text{AII}$ symmetry class), which corresponds to $M_1 = \gamma_0$, $T_l = U \delta_{l,1}$, and one of the chiral disorders preserving time-reversal symmetry $T M_l^T T = M_l$ with matrices $M_l \in \{i\gamma_{1,2}\gamma_3, i\gamma_{1,2}\gamma_5\}$ describing intervalley scattering of fermions in each of the sublattices ($\gamma_5 = -\gamma_0 \gamma_1 \gamma_2 \gamma_3$), $T_l = U/4$. Although realistic impurities yield in fact both these types of disorder (see, e.g., Ref. 4), for theoretical analysis it is informative to consider these types separately. The flow for these types of disorder at the scales $\Lambda \gg |\text{Im}\Sigma|/v_F$, i.e., in the ballistic regime, when one can neglect the quasiparticle damping, was discussed in detail in Ref. 4 (see also references therein). In particular, both disorders γ_0 and $i\gamma_{1,2}\gamma_{3,5}$ yield the flow of the coupling constants to the strong-coupling regime. For our numerical calculations we use the parameters $U^2 n_{\text{imp}}/v_F^2 = 0.8$, $\Lambda_{\text{uv}} = 2$. The corresponding SCBA damping is $\Gamma = 7.76 \times 10^{-4} v_F$. The results of our fRG analysis are presented in Figs. 2–5.

For γ_0 (long-range diagonal) disorder we find saturation of the density of states and imaginary part of the self-energy at values, which are much larger than the SCBA results (see Fig. 2). This agrees with the earlier observation in Ref. 4 that the critical scale of the divergence of vertices in the standard RG analysis Λ_{min} differs from the SCBA result (5) by a factor of 2 in the exponent (for the considered parameters we find $\Lambda_{\text{min}} \simeq 0.04$). The present analysis yields, however, finite vertices at and below the critical scale Λ_{min} (Fig. 3). This is due to the cutoff of the divergence of vertices in the present

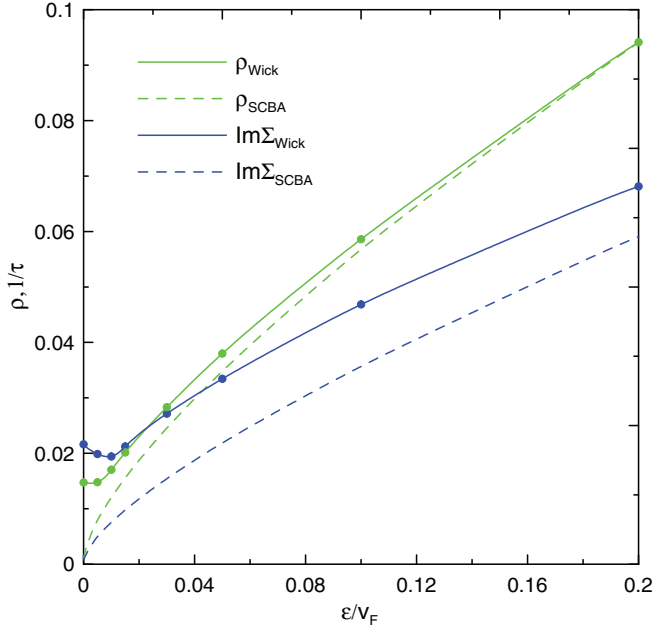


FIG. 2. (Color online) The imaginary part of the self-energy and the density of states (in units of v_F) at different energy distances to the neutrality point for long-range diagonal disorder.

approach by the quasiparticle damping, which occurs since renormalization of the vertices involves dressed rather than bare Green's functions and reflects the nonperturbative character of the considered approach (cf. the flow into the magnetic, superconducting, or charge-ordered phases within the one-particle functional renormalization-group approach¹⁷). From a field-theoretic point of view, this corresponds to an account of many-loop diagrams within the considered truncation of fRG hierarchy. Using SCBA self-energy as an input of fRG flow in the present approach allows us to treat these self-energy effects more efficiently, since vertices do not grow strongly already from the beginning of the flow. The finiteness of the vertices

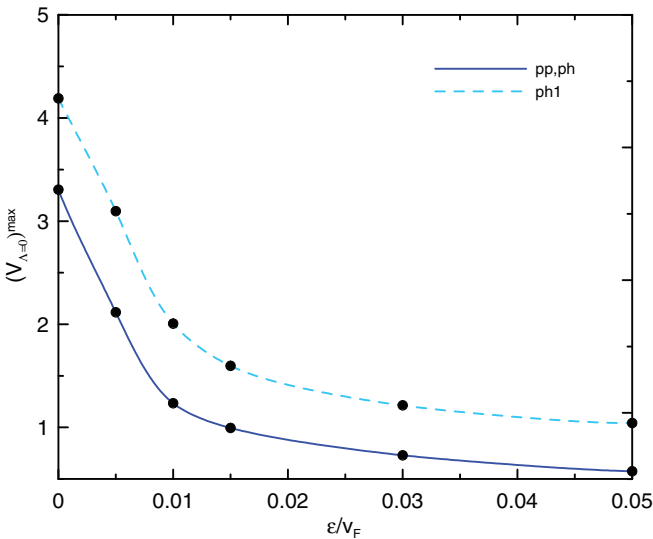


FIG. 3. (Color online) The maximal interaction vertex in the end of the fRG flow as a function of the energy distance to the neutrality point for long-range diagonal disorder.

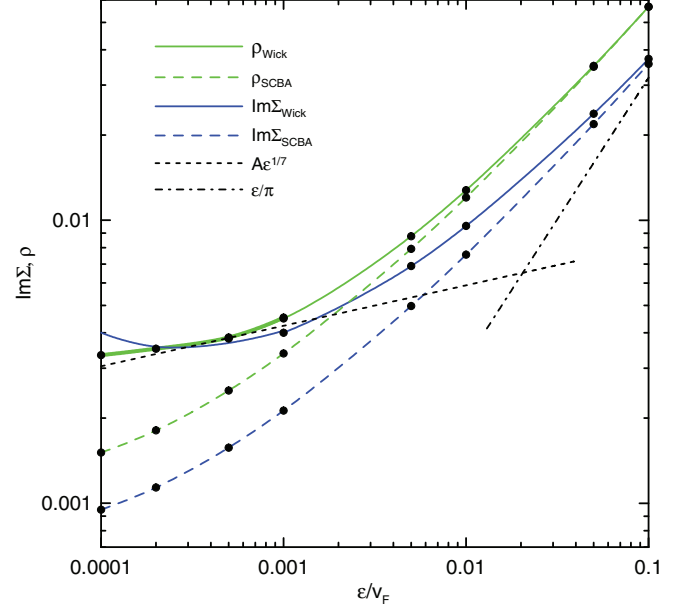


FIG. 4. (Color online) The same as Fig. 2 for chiral disorder of CI symmetry class.

(whose divergences are cut at the quasiparticle damping) allows us to describe the crossover between the ballistic ($|\varepsilon| \gg |\text{Im}\Sigma|$) and the diffusive ($|\varepsilon| \ll |\text{Im}\Sigma|$) regimes at the energy $\varepsilon_{\text{cross}} \simeq 0.02v_F \sim \Lambda_{\text{min}}v_F$ and obtain the density of states and quasiparticle lifetime near the neutrality point. In particular, the quasiparticle damping approaches a value which is approximately equal to the crossover scale $\varepsilon_{\text{cross}}$.

For $i\{\gamma_{1,2}\gamma_{3,5}\}$ disorder we find much smaller values of the electronic damping than for the diagonal disorder (Fig. 4). Moreover, at low energies, the logarithm of the density of states scales almost linearly with $\ln \varepsilon$, with the slope, which is much smaller than for the SCBA result. The slope of the low-energy region agrees well with that obtained in the strong-coupling analysis of the problem,⁸ revealing that the density of states is expected to behave as $\rho \sim \varepsilon^{1/7}$ at small energies; for the exponent we obtain in the present approach a value of 0.1. The

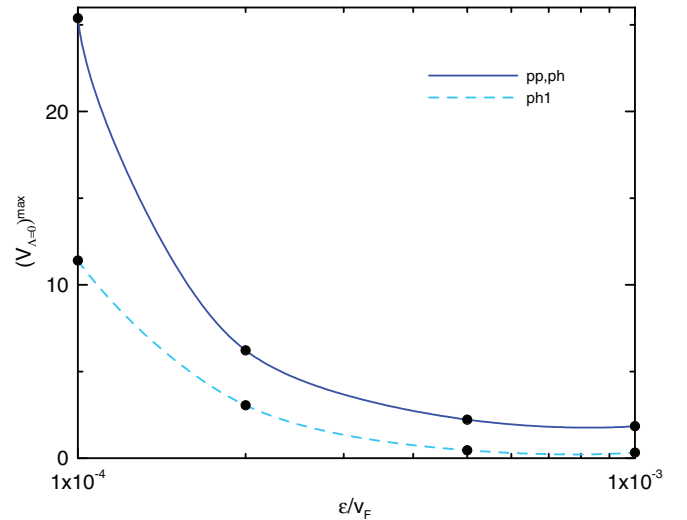


FIG. 5. (Color online) The same as Fig. 3 for chiral disorder of the CI symmetry class.

values of the maximal vertices, obtained for the considering chiral disorder, are shown in Fig. 5 and grow on approaching the neutrality point. This behavior of the vertices is similar to that found for certain symmetries of the disorder in d -wave superconductors in Ref. 18, and is related to approaching chiral symmetry of the considered model at $\varepsilon = 0$, which implies poles in the diffusons and cooperons in a retarded-retarded (RR) channel. The obtained momentum dependence of $V^{\varepsilon\varepsilon,ph}(\mathbf{k})$ at $\varepsilon > 0$ has, however, a maximum at $k \sim |\text{Im}\Sigma|/v_F$ and approaches the corresponding dependence in the retarded-advanced (RA) channel only for very small $\varepsilon < 10^{-4}v_F$. As discussed in Ref. 18, the singularity of the RR diffusons provides peculiarities of the density of states, which is likely related to the observed power law behavior of the DOS for CI symmetry.

In conclusion, we have considered the effect of weak impurities on the electronic properties of graphene. For long-range disorder, we find saturation of the density of states at values which are much bigger than those obtained previously within

the SCBA analysis. On the other hand, for chiral impurities of the CI symmetry class we find indications of a vanishing density of states at the Fermi level, with the power law, which approximates the previously obtained result $\rho \propto \varepsilon^{1/7}$. The functional renormalization-group approach allows one to describe the crossover from the ballistic to the diffusive regime in both cases. For realistic impurities, both long-range and chiral components are present. We expect that the long-range component will be dominant in this case. The qualitative behavior of the density of states in this case agrees with the recent experimental results.²

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¹⁵See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.88.241401> for the analytical form of the fRG equations.

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